

=> b reg
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STRUCTURE FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9
 DICTIONARY FILE UPDATES: 13 SEP 2007 HIGHEST RN 947061-18-9

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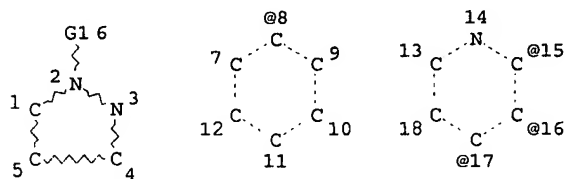
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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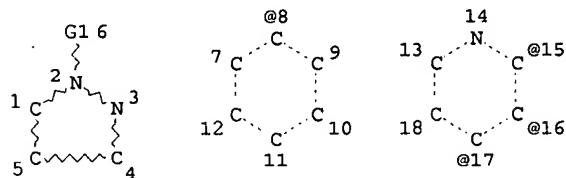
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 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
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 SEARCH TIME: 00.00.02

239539 ANSWERS

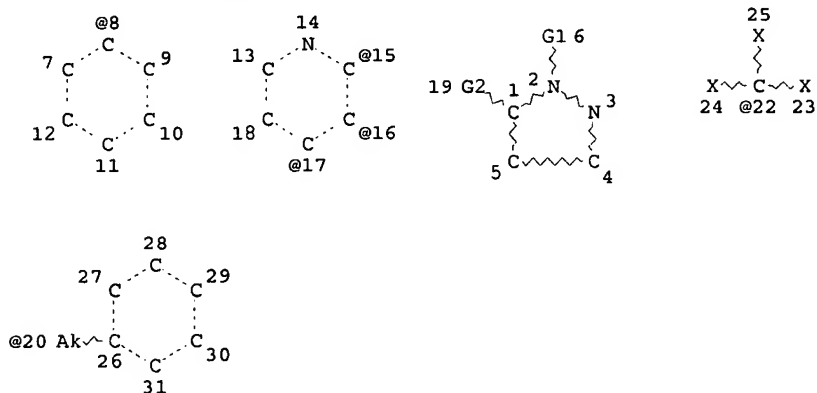
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STEREO ATTRIBUTES: NONE

L5 239539 SEA FILE=REGISTRY SSS FUL L3
L11 STR

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VAR G2=AK/20/CB/22

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DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X5 C AT 20

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STEREO ATTRIBUTES: NONE

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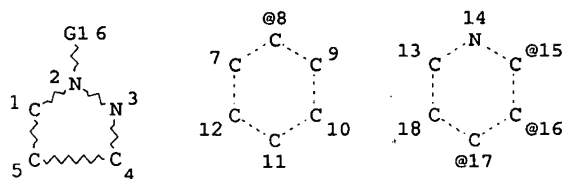
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59980 ANSWERS

SEARCH TIME: 00.00.03

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DEFAULT ECLEVEL IS LIMITED

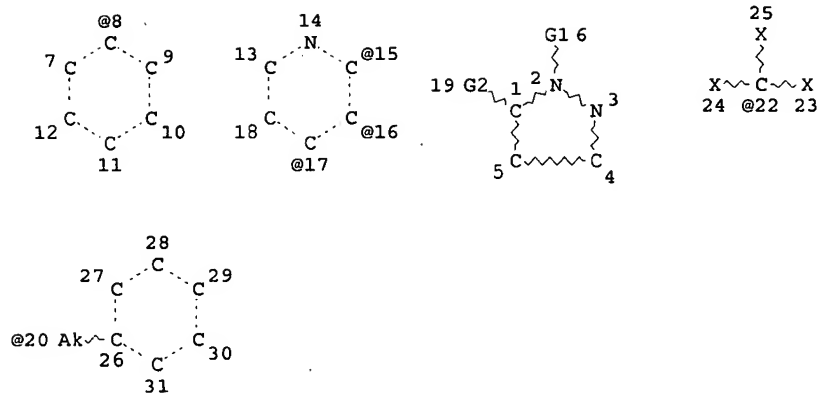
GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

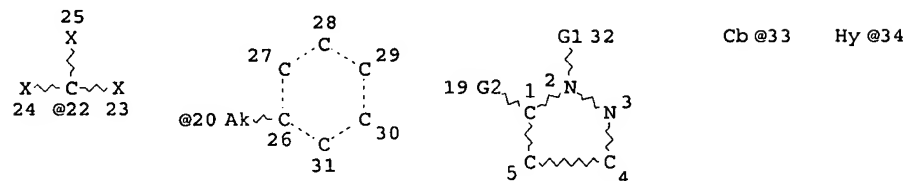
L5 239539 SEA FILE=REGISTRY SSS FUL L3
L11 STR



VAR G1=8/15/16/17
 VAR G2=AK/20/CB/22
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 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS M1-X5 C AT 20

GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE
 L13 59980 SEA FILE=REGISTRY SUB=L5 SSS FUL L11
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VAR G1=33/34
 VAR G2=AK/20/CB/22
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 ECOUNT IS M1-X5 C AT 20
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GRAPH ATTRIBUTES:
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 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
 L16 30343 SEA FILE=REGISTRY SUB=L13 SSS FUL L14

100.0% PROCESSED 59980 ITERATIONS
 SEARCH TIME: 00.00.01

30343 ANSWERS

=> b hcap
 FILE 'HCAPLUS' ENTERED AT 18:10:34 ON 14 SEP 2007
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FILE COVERS 1907 - 14 Sep 2007 VOL 147 ISS 13
FILE LAST UPDATED: 13 Sep 2007 (20070913/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d bib abs fhitr 119 1-2

L19 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:841775 HCAPLUS

DN 141:350163

TI Preparation of arylpyrazoles as serotonin 5-HT_{2A} and 5-HT_{2C} receptor antagonists

IN Schiemann, Kai; Ackermann, Karl-August; Arlt, Michael; Finsinger, Dirk; Schadt, Oliver; Van Amsterdam, Christoph; Bartoszyk, Gerd; Seyfried, Christoph

PA Merck Patent GmbH, Germany

SO Ger. Offen., 102 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE--10315572	A1	20041014	2003DE-1015572	20030405
	AU2004228120	A1	20041021	2004AU-0228120	20040308
	CA---2521201	A1	20041021	2004CA-2521201	20040308
	WO2004089931	A1	20041021	2004WO-EP02353	20040308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP---	1626967	A1	20060222	2004EP-0718277	20040308
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR2004009164	A	20060411	2004BR-0009164	20040308	
CN---	1768051	A	20060503	CN 2004-80008572	20040308
JP2006522035	T	20060928	2006JP-0504584	20040308	
US2006264419	A1	20061123	2005US-0552065	20051005	
PRAI	2003DE-1015572	A	20030405		
	2004WO-EP02353	W	20040308		
OS	MARPAT 141:350163				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Preparation of title compds. I [X = CH, N; R₁ = H, halo, (CH₂)_nHet, etc.; R₂ = (CH₂)_nHet, (CH₂)_nAr, cycloalkyl, etc.; R₃, R₄ = H, (CH₂)_nCOHet, CHO, etc.; n = 0-5; Ar = (un)substituted Ph; Het = (un)substituted monoarom., bicyclic-heterocycle] and their pharmaceutically acceptable salts were prepared. For example, sodium triacetoxyborohydride mediated reductive amination of 1-methyl-piperazine and aldehyde II, e.g., prepared from 2-fluoro- α,γ -dioxo-benzenebutanoic Et ester in 4-steps, afforded the dihydrochloride salt of arylpyrazole III. In 5-HT_{2A} receptor

binding assays, 167-examples of compds. I exhibited IC50 values ranging from 0.015-4.7x10-7M. Compds. I are claimed suitable as ligands of 5-HT receptors.

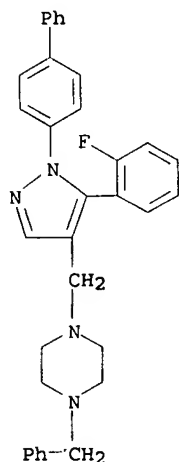
IT 508219-09-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of arylpyrazoles as serotonin 5-HT2A and 5-HT2C receptor antagonists)

RN 508219-09-8 HCAPLUS

CN Piperazine, 1-[[1-[1,1'-biphenyl]-4-yl-5-(2-fluorophenyl)-1H-pyrazol-4-yl]methyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



L19 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:841772 HCAPLUS

DN 141:332186

TI Preparation of arylpyrazoles as serotonin 5-HT2A and/or 5-HT2C receptor antagonists.

IN Schadt, Oliver; Arlt, Michael; Finsinger, Dirk; Schiemann, Kai; Van Amsterdam, Christoph; Bartoszyk, Gerd; Seyfried, Christoph

PA Merck Patent GmbH, Germany

SO Ger. Offen., 78 pp.

CODEN: GWXXBX

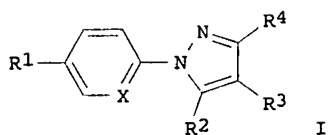
DT Patent

LA German

FAN.CNT 1

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PI	DE--10315569	A1	20041014	2003DE-1015569	20030405
	AU2004228124	A1	20041021	2004AU-0228124	20040310
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	WO2004089932	A1	20041021	2004WO-EP02453	20040310
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	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	CN---1768052	A	20060503	CN 2004-80008603	20040310
	JP2006522039	T	20060928	2006JP-0504620	20040310
	AT---364601	T	20070715	2004AT-0718926	20040310
	US2007010531	A1	20070111	2005US-0552064	20051005

PRAI 2003DE-1015569 A 20030405
 2004WO-EP02453 W 20040310
 OS MARPAT 141:332186
 GI



AB Title compds. [I; R1 = H, A, halo, (CH2)nAr, cycloalkyl, CF3, NO2, cyano, C(NH)NOH, OCF3; R2 = (CH2)nHet, (CH2)nAr, cycloalkyl, CF3; R3, R4 = H, (CH2)nCO2R5, (CH2)nCOHet, CHO, (CH2)nOR5, (CH2)nHet, CH:NOA, etc.; R5 = H, A; A = alkyl, alkoxy, alkenyl, alkoxyalkyl; Ar = (substituted) Ph; Het = (aromatic) mono- or bicyclic heterocyclyl, heteroatom-containing organic residue; X = N, CH; with provisos], were prepared. Thus, [1-(4'-fluorobiphen-4-yl)-5-furan-2-yl-1H-pyrazol-4-ylmethyl]methyl(1-methylpyrrolidin-3-yl)amine showed 5-HT2A activity with IC50 = 5.14E-10.

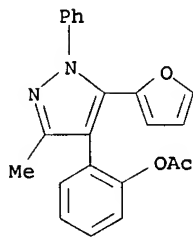
IT 380652-94-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of arylpyrazoles as serotonin 5-HT2A and/or 5-HT2C receptor antagonists)

RN 380652-94-8 HCAPLUS

CN Phenol, 2-[5-(2-furanyl)-3-methyl-1-phenyl-1H-pyrazol-4-yl]-, acetate (ester) (9CI) (CA INDEX NAME)



=> d bib abs hitstr l19 3

L19 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 2003:279562 HCAPLUS

DN 138:304276

TI Preparation of pyrazoles as glycine transporter protein inhibitors for the treatment of neurodegenerative diseases

PA Merck Patent G.m.b.H., Germany; Yamanouchi Pharmaceutical Co.

SO Ger. Offen., 62 pp.

CODEN: GWXXBX

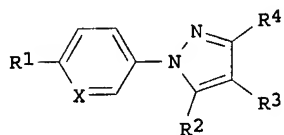
DT Patent

LA German

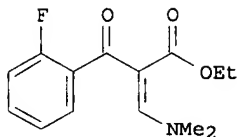
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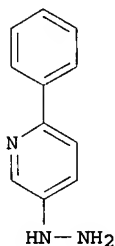
PRAI 2001DE-1049370 A 20011006
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 OS MARPAT 138:304276
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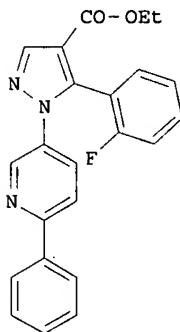
I



II



III



IV

AB Title compds. I [X = CH, N; R1 = H, A, halo, etc.; R2 = Ph, p-chlorophenyl; R3, R4 = H, (CH2)nCO2R5, CHO, etc.; R5 = H, A; A = alkyl, alkenyl, alkoxyalkyl, etc.; n = 0-5] and their pharmaceutically acceptable salts were prepared. For example, condensation of enamine II e.g., prepared from 1,1-dimethoxy-N,N-dimethylmethanamine and 2-fluoro-β-oxo-benzenepropanoic acid Et ester, and aryl hydrazine III, e.g., prepared from 2-chloro-5-nitropyridine in 3-steps, provided pyrazole IV (no yield provided). In glycine transporter protein inhibition studies, approx. 71-examples of compds. I exhibited IC50 values ranging from 0.15 - 8.7 μM, e.g., the IC50 value of pyrazole IV = 2.5 μM. Compds. I are claimed useful for the treatment of schizophrenia, depression, dementia, etc.

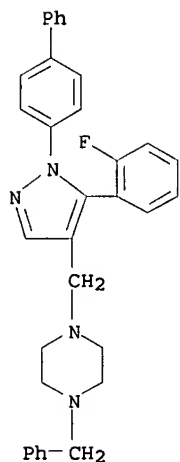
IT 508219-09-8P 508219-31-6P, 4-[2-[1-Biphenyl-4-yl-5-(2-fluorophenyl)-1H-pyrazol-4-yl]-ethyl]morpholine

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrazoles as glycine transporter protein inhibitors for the treatment of neurodegenerative diseases)

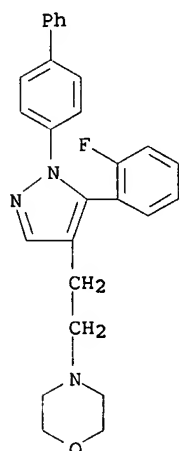
RN 508219-09-8 HCAPLUS

CN Piperazine, 1-[[1-[1,1'-biphenyl]-4-yl-5-(2-fluorophenyl)-1H-pyrazol-4-yl]methyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 508219-31-6 HCAPLUS

CN Morpholine, 4-[2-[1-[1,1'-biphenyl]-4-yl]-5-(2-fluorophenyl)-1H-pyrazol-4-yl]ethyl]- (9CI) (CA INDEX NAME)



=> b hcap

FILE 'HCAPLUS' ENTERED AT 18:46:36 ON 14 SEP 2007

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FILE COVERS 1907 - 14 Sep 2007 VOL 147 ISS 13

FILE LAST UPDATED: 13 Sep 2007 (20070913/ED)

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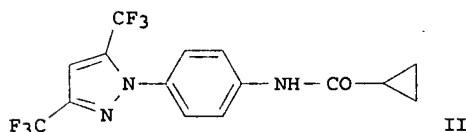
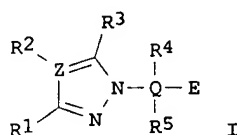
This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d bib abs hitstr 136 tot

L36 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
 AN 2001:851793 HCAPLUS
 DN 136:5986
 TI Preparation of azole inhibitors of cytokine production
 IN Bamaung, Nwe Y.; Basha, Anwer; Djuric, Stevan W.; Gubbins, Earl J.; Luly, Jay R.; Tu, Noah P.; Madar, David J.; Warrior, Usha; Wiedeman, Paul E.; Zhou, Xun; Sciotti, Richard J.; Wagenaar, Frank L.
 PA USA
 SO U.S. Pat. Appl. Publ., 124 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

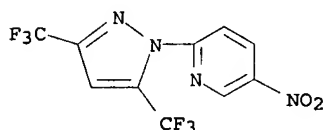
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PI	US2001044445	A1	20011122	1999US-0289155	19990408
PRAI	1999US-0289155		19990408		
OS	MARPAT 136:5986				
GI					



AB The title compds. [I; R1, R3 = H, aryl, perfluoroalkyl, etc.; Z = N, C; R2 is absent or = H, alkyl, cycloalkyl, etc.; Q = (hetero)aryl (when Q = Ph, the Ph is 2-, 3-, or 4-substituted by E relative to the position of attachment of the pyrazole or 1,2,4-triazole ring to the Ph ring); R4, R5 = H, alkyl, haloalkyl, etc.; E = NO2, NH2, etc.], useful for inhibiting cytokine (Interleukin-2, Interleukin-4, or Interleukin-5) production and cellular proliferation in stimulated human T cell lines or human peripheral blood mononuclear cells (biol. data given) and therefore have utility in the treatment of diseases that are prevented by or ameliorated with cytokine inhibitors, were prepared General procedures for preparation of compds. I were described. Thus, the title compound II was prepared

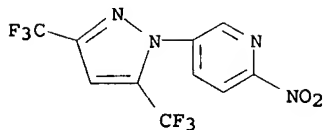
IT 245748-05-4P 245748-10-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of azole inhibitors of cytokine production)

RN 245748-05-4 HCAPLUS
 CN Pyridine, 2-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]-5-nitro- (9CI) (CA INDEX NAME)



RN 245748-10-1 HCAPLUS
 CN Pyridine, 5-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]-2-nitro- (9CI) (CA

INDEX NAME)



L36 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:659365 HCAPLUS

DN 131:271873

TI Preparation of pyrazoles and triazoles as inhibitors of cytokine production

IN Ba Maung, Nwe Y.; Basha, Anwer; Djuric, Stevan W.; Gubbins, Earl J.; Luly, Jay R.; Tu, Noah P.; Madar, David J.; Warrior, Usha; Wiedeman, Paul E.; Zhou, Xun; Wagenaar, Frank L.; Sciotti, Richard J.

PA Abbott Laboratories, USA

SO PCT Int. Appl., 319 pp.

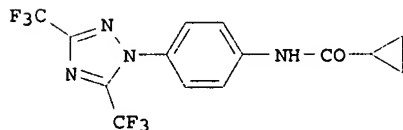
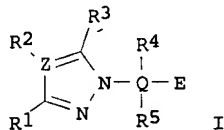
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

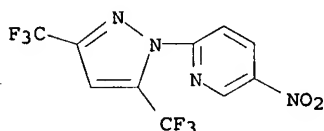
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WO---9951580	A1	19991014	1999WO-US07766	19990408
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA---2327185	A1	19991014	1999CA-2327185	19990408
AU---9933879	A	19991025	1999AU-0033879	19990408
EP---1068187	A1	20010117	1999EP-0915341	19990408
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JP2002510679	T	20020409	2000JP-0542301	19990408
MX2000PA09837	A	20010405	2000MX-PA09837	20001006
PRAI 1998US-0056996	A	19980408		
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OS MARPAT 131:271873				
GI				



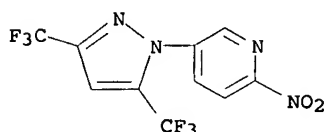
AB Title compds. [I; R1 = H, NH2, OCONH2, CN, NO2, OH, CO2H, F, Cl, Br, I, aryl, perfluoroalkyl, heterocyclyloxy, heterocyclylsulfonyl; R2 = H, alkyl, cycloalkyl, alkylcarbonyl, heterocyclyl; R3 = H, NH2, OCONH2, CN, NO2, OH, CO2H, F, Cl, Br, I, aryl, perfluoroalkyl, heterocyclyloxy, heterocyclylsulfonyl; R4 and R5 are independently selected from H, alkyl, alkoxy, halo, perfluoroalkyl, CN, heterocycle; E = LB; B = alkyl, alkenyl, alkynyl; L = N:N, N:CH, CH:N, ON:CH, O, CO, NH, NHCO, NHSO2, NHCH2,

alkenylene; Q = benzene ring with 2, 3, or 4 substituted E, heterocycle; Z = C; R2Z = N], E, Z isomers, stereoisomers, pharmaceutical acceptable salts, and prodrugs are prepared and tested as cytokine production inhibitors and are useful for treating diseases that are prevented by or ameliorated with Interleukin-2, Interleukin-4, or Interleukin-5 production inhibitors. Thus, the title compound II was prepared

IT 245748-05-4P 245748-10-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of pyrazoles and triazoles as inhibitors of cytokine production)
 RN 245748-05-4 HCAPLUS
 CN Pyridine, 2-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]-5-nitro- (9CI) (CA INDEX NAME)



RN 245748-10-1 HCAPLUS
 CN Pyridine, 5-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]-2-nitro- (9CI) (CA INDEX NAME)



RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> b uspatall
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 CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATOLD' ENTERED AT 18:47:05 ON 14 SEP 2007
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FILE 'USPAT2' ENTERED AT 18:47:05 ON 14 SEP 2007
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=> d bib abs hitstr 138 tot

L38 ANSWER 1 OF 1 USPATFULL on STN
 AN 2001:212449 USPATFULL
 TI AZOLE INHIBITORS OF CYTOKINE PRODUCTION
 IN BAMAUNG, NWE Y., NILES, IL, United States
 BASHA, ANWER, LAKE FOREST, IL, United States
 DJURIC, STEVAN W., LIBERTYVILLE, IL, United States
 GUBBINS, EARL J., LIBERTYVILLE, IL, United States
 LULY, JAY R., WELLESLEY, MA, United States
 TU, NOAH P., GURNEE, IL, United States
 MADAR, DAVID J., GRAYSLAKE, IL, United States
 WARRIOR, USHA, GREEN OAKS, IL, United States
 WIEDEMAN, PAUL E., LIBERTYVILLE, IL, United States
 ZHOU, XUN, PARK CITY, IL, United States
 SCIOTTI, RICHARD J., GURNEE, IL, United States
 WAGENAAR, FRANK L., GURNEE, IL, United States
 PI US-20010044445 A1 20011122
 AI 1999US-000289155 A1 19990408 (9)
 DT Utility
 FS APPLICATION
 LREP ABBOTT LABORATORIES, DEPT. 377 - AP6D-2, 100 ABBOTT PARK ROAD, ABBOTT PARK, IL, 60064-6050
 CLMN Number of Claims: 44
 ECL Exemplary Claim: 1
 DRWN No Drawings

LN.CNT 9955

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds having the formula ##STR1##

are useful for treating diseases that are prevented by or ameliorated with Interleukin-2, Interleukin-4, or Interleukin-5 production inhibitors.

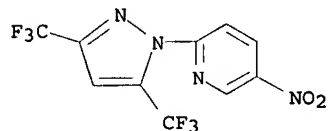
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 245748-05-4P 245748-10-1P

(preparation of azole inhibitors of cytokine production)

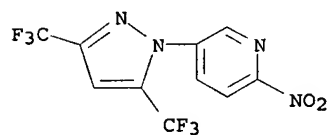
RN 245748-05-4 USPATFULL

CN Pyridine, 2-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]-5-nitro- (9CI) (CA INDEX NAME)



RN 245748-10-1 USPATFULL

CN Pyridine, 5-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]-2-nitro- (9CI) (CA INDEX NAME)



=> d his

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L2 50 L1
L3 STR L1
L4 50 L3
L5 239539 L3 FULL

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L6 1 US20070010531/PN

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L9 170 L5 AND L8

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L12 50 L11 SAM SUB=L5
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SAV TEM L13 J064C1/A
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SAV TEM L5 J064C1B/A
L17 47 L16 AND L8

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L19 3 L10,L18
L20 1 L19 AND GLYCINE/TI
SEL HIT RN

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L21 2 E1-2
L22 1 PYRIDINE/CN
L23 4936 46.156.30/RID AND L16

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L27 STR L14
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L30 27954 L16 NOT L29

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L33 148 L32 AND PD<=20000310
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L35 2 C10H4F6N4O2 AND L34

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